UNIVERSITY OF JOHANNESBURG

FACULTY OF SCIENCE
FAKULTEIT NATUURWETENSKAPPE

DEPARTMENT OF PHYSICS
DEPARTEMENT FISIKA

APK

PHY003B

STATISTICAL AND SOLID STATE PHYSICS

NOVEMBER 2014

DATE 01 NOVEMBER 2014	**SESSION 08:30 – 11:30**
INTERNAL MODERATOR	**PROF G.R. HEARNE**
EXTERNAL MODERATOR	**PROF W. MEYER (UP)**
DURATION 3 HOURS	**MARKS 120**

THIS PAPER CONSISTS OF 12 PAGES INCLUDING THIS COVER

Instructions

ANSWER ANY FOUR OUT OF
FIVE QUESTIONS FROM EACH SECTION
(eight questions in total)

QUESTION A1 follows /…

Section A : STATISTICAL MECHANICS

QUESTION A1 **[15]**

A perfect classical gas of a fixed number of molecules N contained in a fixed volume V is in contact with a heat bath at temperature T. Each molecule has a discrete set of energy states $\varepsilon_1 \leq \varepsilon_2 \leq \varepsilon_3 \leq \ldots\ldots\varepsilon_n$. First indicate what the single-particle partition function, Z_1 , is. Then with a critical discussion of the relevant physics, which one of the following expressions is appropriate to use for the partition function Z for the N molecules :

$$Z \ (T,V,N) = (Z_1)^N$$

OR

$$Z \ (T,V,N) = \frac{1}{N!}(Z_1)^N .$$

In answering this question you should firstly formulate the case of 2 molecules in the enclosure before giving a general formulation. Furthermore, the meaning of the terms perfect and classical and its implications to the present problem should be clarified in your answer.

QUESTION A2 **[15]**

Depart from the partition function for a perfect quantal gas

$$Z(T,V,N) = \sum_{n1,n2..} \exp\{-\beta \sum_r n_r \varepsilon_r\}$$

where the summation refers to all possible sets $\{n_1, n_2, n_3 \ldots\}$ of occupation of single-particle energy states $\{\varepsilon_1, \varepsilon_2, \varepsilon_3 \ldots\}$. Derive an expression for the partition function Z_{ph} as well as an expression for the mean occupation number $\overline{n_i}$ for photons radiated in a Blackbody cavity at temperature *T*. Furthermore assume the relation $\overline{n_i} = -\frac{1}{\beta}\frac{\partial \ln Z_{ph}}{\partial \varepsilon_i}$ to find Planck's result for the mean occupation number

$$\overline{n_i} = \frac{1}{e^{\beta\varepsilon_i} - 1}$$

in terms of $(\beta = 1/k_B T)$ and ε_i. Fully motivate the physics behind your calculations, especially in obtaining Z_{ph}.

A photon has energy and momentum $\varepsilon = \hbar\omega$ and $p = \varepsilon / c$, respectively. The general expression for the density of momentum states is

$$f(p)\,dp = \frac{V\, 2 \times 4\pi p^2 dp}{h^3} .$$

Describe qualitatively the steps you would follow to arrive at Planck's radiation law for the energy density in the cavity :

$$U(\omega,T)d\omega = \frac{\hbar\omega^3\, d\omega}{\pi^2 c^3 \left(\exp(\beta\hbar\omega) - 1\right)} .$$

Note , that a detailed derivation of this equation is NOT required.

QUESTION A3 **[15]**

The diatomic molecules of a certain gas, each with a moment of inertia I have rotational energy levels given by

$$\varepsilon_l = \frac{\hbar^2 l(l+1)}{2I} \quad l = 0,1,2,...$$

with degeneracy $g_l=(2l+1)$.

(a) Show that the one-body rotational partition function Z_1, is given by

$$Z_1 = 1 + 3\exp\left(-\hbar^2 \big/ (I\, k_B T)\right)$$

in the low temperature limit, $T \ll \dfrac{\hbar^2}{k_B I}$. Show that in the high temperature limit ,

$$Z_1 = \frac{2\, I\, k_B T}{\hbar^2}.$$

In the high temperature limit the summation over l may be replaced by an integral (why ?) which may then be evaluated by the substitution $x= l(l+1)$.

(b) Recall that the internal energy *E* is related to the partition function through

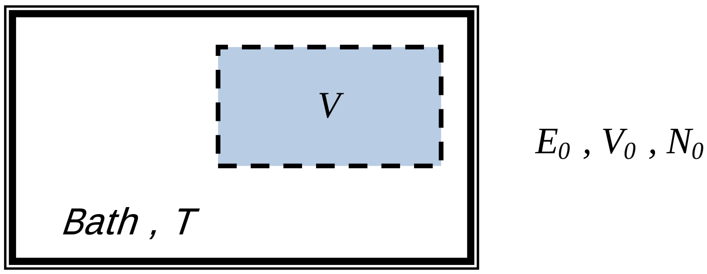
$$\overline{E} = -\frac{\partial \ln(Z_N)}{\partial \beta},$$ where Z_N is the *N*-particle partition function.

Calculate the rotational contribution to the internal energy of one mole of N_2 at 20 °C, given that I = 1.42×10^{-46} kg m^2. You first have to decide whether to use the high or low temperature limits of Z_1 above and also consider what is Z_N .

Information : $\hbar$=1.055 ×10^{-34} J s , k_B=1.381×10^{-23} J K^{-1} R=8.314 J K^{-1} mol^{-1} N_A=6.02×10^{23} mol^{-1}

QUESTION A4 **[15]**

Consider a system of fixed volume in contact with a heat bath , it can exchange particles and energy with the heat bath. If the system has N particles it can possess a sequence of energies (microstates) $E_{N1} \leq E_{N2} \leq E_{N3} \leq \ldots$.



The total energy, volume and number of particles of the composite system is fixed at E_0, V_0 *and* N_0, respectively. Show that the probability of the system being in energy state E_{Nr} when it has N particles is given by the Gibbs (grand canonical) distribution

$$P_{Nr} = \frac{\exp\left[-\beta\left(E_{Nr} - \mu N\right)\right]}{\mathbf{Z}} .$$

The grand partition function is

$$\mathbf{Z} = \sum_{N=0}^{\infty} \sum_{r=1}^{\infty} \exp\left[-\beta\left(E_{Nr} - \mu N\right)\right],$$

and $N = \sum_i n_i$ *and* $E_{Nr} = \sum_i n_i \varepsilon_i$ when the subscript i refers to ***single particle energy states*** ε_i. The quantity $\mu = \partial E_{bath} / \partial N_0$ is the chemical potential. The derivation is similar to what you did for the Boltzmann distribution. Explain the reasoning of each of your steps in the derivation.

<u>QUESTION A5</u> **[15]**

For a Bose gas the number of momentum states between *p* and *p + dp* is :

$$f\left(p\right)dp = \frac{V\,4\pi\,p^2 dp}{h^3}\ .$$

The dispersion relation and Bose-Einstein distribution, respectively, are given by :

$$\varepsilon = \frac{p^2}{2m}; \qquad \overline{n}_\varepsilon = \frac{1}{\exp[\beta(\varepsilon-\mu)]-1} \quad .$$

Suppose the Bose gas has *N* particles. Derive the following expression and explain why it is an indication of the number of bosons in the excited energy states $\varepsilon > 0$ only, if the ground state is considered as $\varepsilon = 0$:
.

$$N_{exc} = \left[\frac{2\pi V}{h^3}(2m)^{3/2}(k_B T)^{3/2}\int_0^\infty \frac{z^{1/2}dz}{\mathrm{e}^{(z-\beta\mu)}-1}\right] \quad ,$$

where $z = \varepsilon/k_B T = \beta\varepsilon$.

Justify that μ must be negative and furthermore that $|\mu|$ decreases and tends to zero as the temperature is lowered towards $T \rightarrow 0$ K. Then use this to discuss Bose-Einstein condensation and the significance of the critical (condensation) temperature T_C in terms of excited state and ground state occupancies. Derive a final expression for the relation between *N/V* and T_C . Then also discuss the significance of T_C in relation to the de-Broglie wavelength of the Bose particles. You may if needed use the following information :

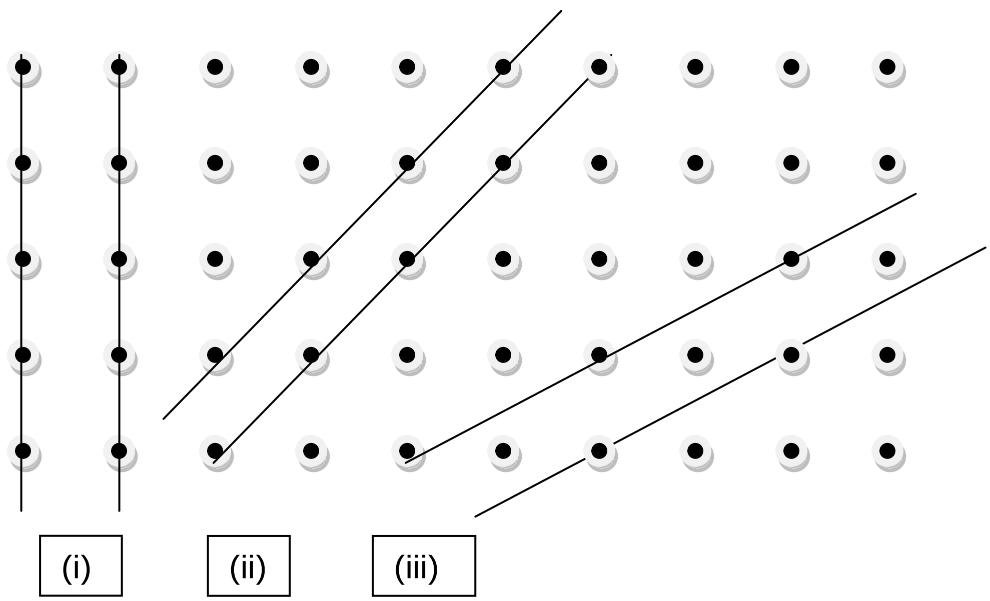
$$\int_0^\infty \frac{z^{1/2}dz}{e^z-1} = \left(\frac{\sqrt{\pi}}{2}\right)\times 2.61,$$

$$\text{de-Broglie wavelength } \lambda_{\mathrm{dB}} = \frac{h}{\sqrt{3mk_B T}}$$

Section B : SOLID STATE PHYSICS

QUESTION B1 **[15]**

(a) Explain what are the Miller indices (h,k,l) and how they are obtained in any Bravais lattice. For the following planes in the 2-D projection of the simple cubic lattice of lattice spacing *a* , show how you obtain the Miller indices for the following sets of planes (i), (ii) and (iii). The planes also extend along the normal into and out of the page, which is the third dimension of the lattice.



(b) Given the real lattice $R = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$ and that it is simple cubic as in (a) above with $\vec{a}_1 = a\hat{i}$; $\vec{a}_2 = a\hat{j}$; $\vec{a}_3 = a\hat{k}$, where the third dimension is not shown. Define what is the reciprocal lattice $\vec{G}$ in terms of lattice vectors $\vec{b}_1$, $\vec{b}_2$, $\vec{b}_3$. Depict this fully labelled reciprocal lattice in your answer book. Show how the diffracting planes in (a) are represented in this reciprocal lattice.

(c) State but do not prove what is the relation between the spacing between the planes in (a) and corresponding reciprocal lattice vectors in (b). Use this expression to find the spacing between the planes (iii) in (a) from this relation. Also state, but do not derive , what is the relation between the orientation of the planes in (a) to that of reciprocal lattice vectors in (b).

<u>QUESTION B2</u> **[15]**

Lattice vibrations on a linear chain of equally spaced atoms with alternate masses (diatomic chain) M and m which are coupled with a spring constant K (nearest–neighbour interactions only) are described by travelling – wave solutions

$$u_n = A\exp\left[i\left(k\,x_n^0 - \omega t\right)\right] \text{ and } u_{n-1} = \alpha A\exp\left[i\left(k\,x_{n-1}^0 - \omega t\right)\right].$$

We obtain the following equations relating frequency ω and wave-number k :

$$-\omega^2 M = 2K\left[\alpha\cos\left(\frac{ka}{2}\right) - 1\right] \text{ and}$$
$$-\alpha\omega^2 m = 2K\left[\cos\left(\frac{ka}{2}\right) - \alpha\right].$$

Qualitatively explain how we arrived at these equations. A detailed derivation is <u>no</u>t required.

(a) Assume the preceding results and show that the dispersion relation for the system is given by

$$\omega^2 = \frac{K(M+m)}{Mm} \pm K\left[\left(\frac{M+m}{Mm}\right)^2 - \frac{4}{Mm}\sin^2\left(\frac{1}{2}ka\right)\right]^{\frac{1}{2}}.$$

Sketch and explain features of this dispersion relation associated with the + and – signs separating the two terms of the equation above.

(b) Show that the limiting solutions for this equation in the long wavelength limit lead to

$$\omega^2 = \frac{2K(M+m)}{Mm} \quad \text{or} \quad \omega^2 = \frac{1}{2}\frac{K}{(M+m)}\left(ka\right)^2$$

and show that this leads to α values of $-M/m$ and 1. Interpret these in terms of the dispersion relation you have sketched and depict typical examples of such transverse modes of vibration.

QUESTION B3 **[15]**

The single particle energies of a harmonic oscillator (phonon) mode of vibration is given by $\varepsilon_n = (n + \frac{1}{2})\hbar\omega$.

(a) Set up the partition function Z_1 and show that it can be written as

$$z_1 = \frac{\exp\left(-x/2\right)}{1 - \exp(-x)} \quad \text{where} \quad x = \hbar\omega / k_B T \ .$$

Using $\bar{\varepsilon} = -\dfrac{\partial \ln z_1}{\partial \beta}$, show that

$$\bar{\varepsilon} = \frac{1}{2}\hbar\omega + \frac{\hbar\omega}{\exp\left(\hbar\omega / k_B T\right) - 1} \ .$$

What is this average energy of the oscillator and heat capacity C_V in the high temperature limit ?

Denote $\theta = \dfrac{\hbar\omega}{k_B}$, then show that the heat capacity in the low temperature limit is

$$C_V = k_B \left(\frac{\theta}{T}\right)^2 \exp\left(-\theta / T\right).$$

(b) Briefly comment on why this is considered an Einstein model of lattice vibrations in a solid and how it differs from the Debye model.

QUESTION B4 **[15]**

Show that the kinetic energy of a free electron gas at *0 K* is given by

$$E = \frac{3}{5} N \, \varepsilon_{\mathrm{F}} \, .$$

It is given that the Fermi energy is

$$\varepsilon_F \;=\; \frac{\hbar^2}{2m} \left(3\pi^2 \; \frac{N}{V} \right)^{2/3} ,$$

where N/V is the electron density. The density of energy states is given as

$$g(\varepsilon)\, \mathrm{d}\varepsilon \;=\; \frac{V}{2\pi^2 \hbar^3} \, (2m)^{3/2} \varepsilon^{1/2} \mathrm{d}\varepsilon \, .$$

Also calculate the pressure $P = -\,\partial E / \partial V$ for the electron gas.

QUESTION B5 **[15]**

The Fermi-Dirac distribution function is given by

$$f(\varepsilon) = \frac{1}{\exp\left[(\varepsilon - \mu)/k_B T\right] + 1}$$

It is given that the density of states for the valence band is

$$g(\varepsilon) = \frac{V}{2\pi^2 \hbar^3}(2m_h)^{3/2}(-\varepsilon)^{1/2},$$

with m_h the effective mass of holes in the valence band.

(a) Assuming that the Fermi level is within the gap and not near the band edges, show that the number of holes per unit volume in the valence band at temperature T (thermal excitation of charge carriers) is given by

$$p = 2\left(\frac{2\pi m_h k_B T}{h^2}\right)^{3/2} \exp(-\mu/k_B T).$$

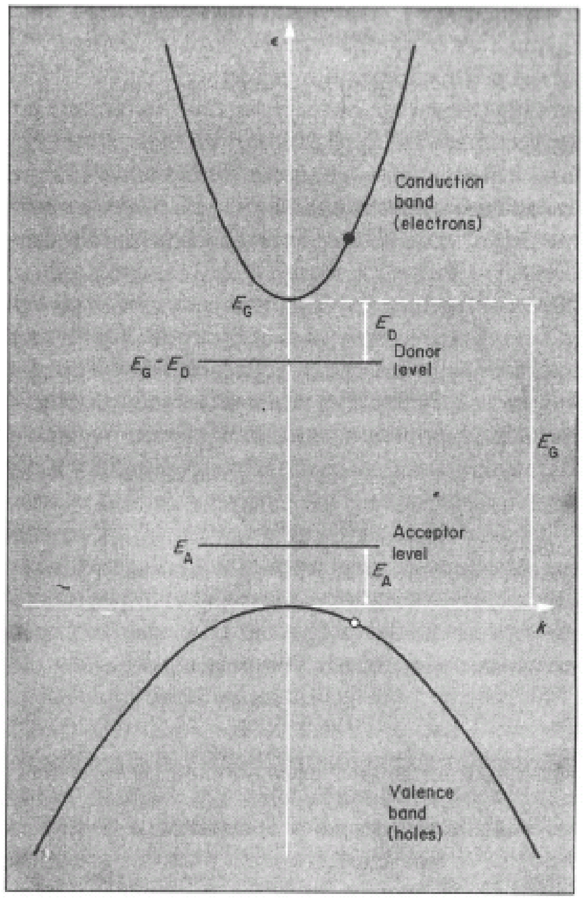
It is given that

$$\int_0^\infty x^{1/2} e^{-ax} dx = \frac{\pi^{1/2}}{2a^{3/2}}.$$

(b) The number of electrons n per unit volume in the conduction band is given by a similar expression $n = 2\left(\frac{2\pi m_e k_B T}{h^2}\right)^{3/2} \exp((\mu - E_G)/k_B T).$

Show for an intrinsic semiconductor that $\mu \approx \frac{1}{2}E_G$, the Fermi level is mid-way in the gap.

Semiconductor : band-structure



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